

AUTOFIT AND THE SPECTRUM OF EUGENOL

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The rotational spectrum of eugenol, the primary constituent in clove oil, was obtained via chirped-pulse Fourier transform microwave spectroscopy from 3-8 GHz in a supersonic expansion on a sample that was extracted from cloves via steam distillation. Ab initio calculations indicate that this molecule possesses several conformers with energies that are only a few hundred wavenumbers above that of the global minimum conformation, due to different relative orientations of the molecule's methoxy and allyl groups. Eugenol's spectrum was analyzed with a new version of the Autofit software that has been designed to run in cluster computing environments. Here we will present the results of this study, including benchmarking results for the new version of Autofit.